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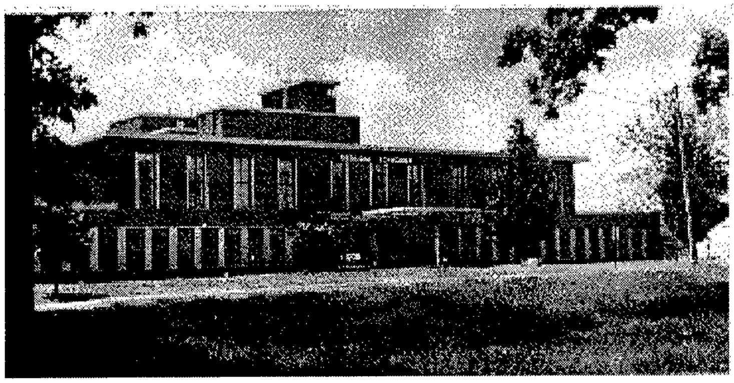
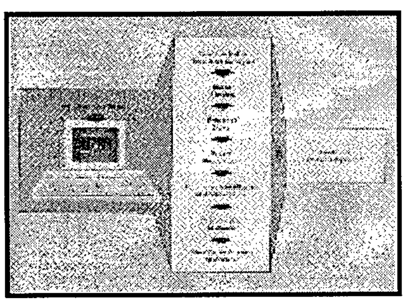


# Adapting Techniques and Materials to Industrial Needs

## Smart Chemical Sensors

The ultimate goal of environmental monitoring is "instantaneous" detection of target analytes. A CMT analytical chemist is designing unique data analysis algorithms for creating "smart" chemical sensors. The term "smart"; means that sensors employing these algorithms would be capable of automated data analysis and decision making.

These algorithms encode into a numerical procedure the visual and logical procedures that an expert uses to analyze sensor data. It does not matter whether the target analyte is a toxic gas or an impurity in a process stream, nor does it matter whether the detection is accomplished by spectroscopic, chromatographic, electrochemical, or radio-chemical methods. Because the algorithms reduce analysis time and analytical costs and can be implemented as part of computer software or hardware, they have tremendous potential in such areas as on-line process control, on-site monitoring, and remote sensing. The resulting smart sensors provide important advantages in multisensor data fusion, in which multiple chemical sensors are connected to a central processing system.

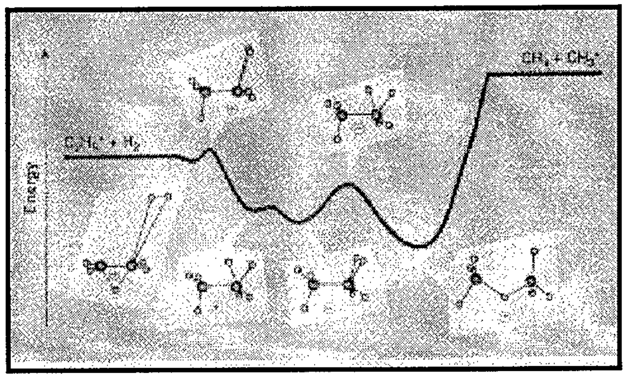


*Schematic for creating smart chemical sensors. Digital filters extract analyte information from background noise and interferences in raw signal. Pattern-recognition procedures make an automated qualitative decision regarding the presence or absence of target analyte. Chemometric methods analyze the filtered data to obtain quantitative data.*

## New Quantum Chemical Method

In collaboration with researchers from AT&T Bell Laboratories and Carnegie Mellon University, a CMT theoretical chemist has developed a new quantum chemical method for calculating the total energies of compounds composed of light elements (atomic numbers 1 through 18). This powerful method, called the Gaussian-2 (G2) quantum chemical code, has led to improved calculated values (within 2 kcal/mole of observed data) for atomization energies, ionization energies, proton affinities, and electron affinities.

The G2 code is now being widely used in universities and industry for the accurate calculation of thermochemical data. It offers tremendous possibilities for identifying new processes and novel materials without the need for exhaustive, unguided laboratory research and has relevance to applications in high-temperature industrial processes, catalysis, chemical synthesis, and assessments of chemical hazards or safety.

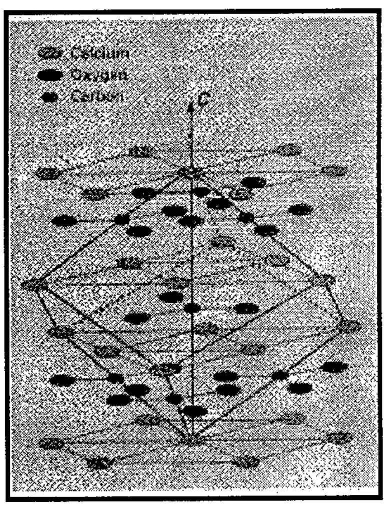


*Calculated changes in potential energy for reaction of $C_2H_5+$ with hydrogen. These G2 calculations are being used in a basic science study of zeolites (microporous crystals of enormous importance to the chemical industry).*

## Mineral-Fluid Interactions in Systems Related to Natural Resources

We have been applying synchrotron radiation techniques to experimental studies of chemical processes occurring at mineral-fluid interfaces (for example, dissolution and precipitation, adsorption, heterogeneous nucleation, recrystallization, oxidation-reduction, solid-state formation, and epitaxial growth). Such processes control geochemical transport, including contaminant migration in groundwater aquifers, and are therefore of practical importance. For this work, we have developed and fabricated an X-ray transparent reaction cell.

This novel device continuously monitors reaction progress as a mineral surface reacts with a fluid. Use of this cell, combined with other sophisticated analytical techniques, is applicable to a wide range of geochemical studies, such as contaminant transport in surface water and groundwater, nutrient cycling in agricultural systems, and compatibility of various industrial byproducts with the natural environment.

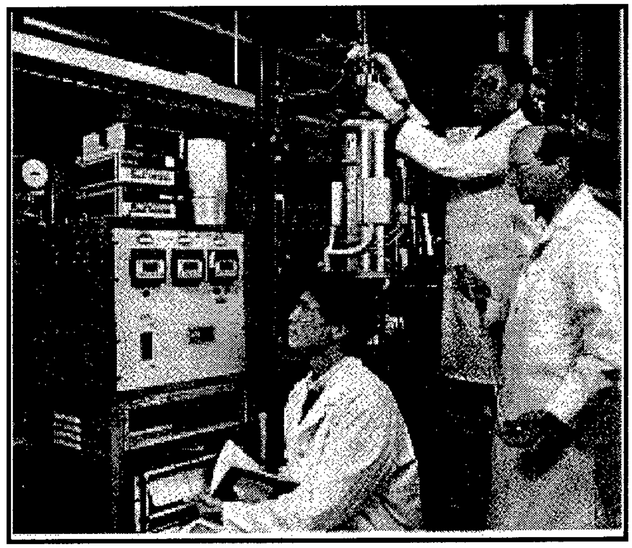


*Crystal structure of calcite showing rhombohedral cleavage surfaces. Such crystals are used in geochemical studies of atomic-scale processes at the interface between rock (calcite) and water. Analyses of this interface are done with synchrotron X-ray techniques.*

## High-Temperature Superconducting Materials

Argonne is a leader in developing a new class of materials called "high-temperature superconductors." These materials are attractive because they lose all electrical resistance when cooled to the temperature of liquid nitrogen (77 degrees above absolute zero). Working with an industrial partner (American Superconductor Corp.), we are developing a method for manufacturing long, durable lengths of superconducting wire made from a composite ceramic material: silver-sheathed $(Bi,Pb)_2Sr_2Ca_2Cu_{3O}x$.

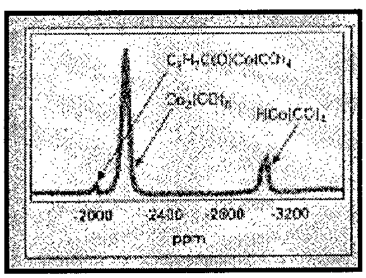
Both thermodynamic and microstructural methods are applied to investigate the phase evolution and microstructure development that take place during composite processing. This high-temperature superconducting product could be used in high-efficiency motors and generators, magnets, energy-storage devices, flywheels with low energy loss, fault-current limiters, and power-transmission lines.



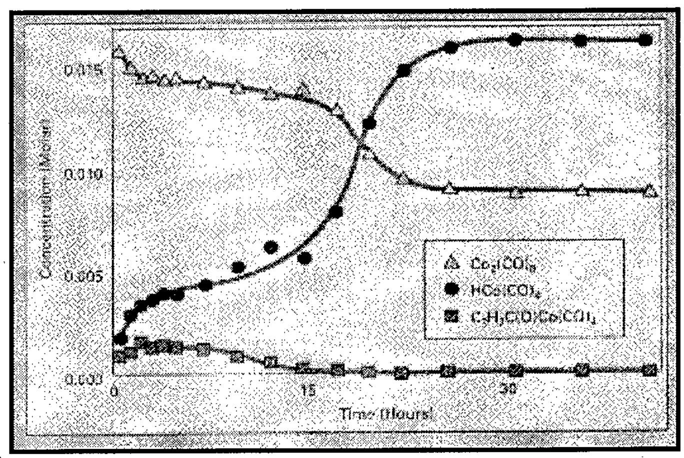
*Testing of silver-sheathed wire prepared with high-temperature superconducting materials.*

## Catalytic Processes for Generating Industrial Chemicals

Advances in basic chemistry research in CMT have led to the discovery of new catalytic processes for converting petroleum-based hydrocarbon feedstocks into alcohols and aldehydes that can be used as industrial solvents (for example, plasticizers), detergents, and agricultural chemicals. This research centers on modifying the commercial oxo processes used for the hydroformylation of olefins, a family of hydrocarbons. The modifications replace conventional separation of the catalytic products by distillation steps with more energy-efficient separations that use Carbon Dioxide in a supercritical fluid. They also make the oxo processes more environmentally benign by achieving cleaner separations and by replacing liquid solvents with relatively nontoxic, nonflammable, and easily recycled Carbon Dioxide gas. If the modified processes are successful, the overall benefits could be large, because the total U.S. hydroformylation capacity exceeds 5 million tons of product per year.




*Concentrations of catalytic intermediates formed during the hydroformylation of propylene in supercritical Carbon Dioxide at 80 degrees C and high pressure. These data were derived from in situ NMR spectra (top graph) of the reacting gas stream over time and are used in studies to improve catalytic processes.*




## High-Resolution NMR Probe for Material Structures

We have developed a relatively inexpensive technique that uses nuclear magnetic resonance (NMR) to probe the structures of ceramics, alloys, composites, and coatings. The new technique, "toroid cavity imaging," provides resolutions up to 100 times better than conventional magnetic resonance imaging. This technique was originally developed for high-pressure NMR studies, especially catalytic reactions that occur at high pressures, but has application in any research area where NMR spectral information is desired as a function of distance. For example, the probe is being used to map electrochemical events emanating radially, within a thin diffusion layer, from an electrode of a high-performance battery designed for an electric vehicle.

*Toroid cavity detector developed for NMR investigations at high temperatures and pressures.*

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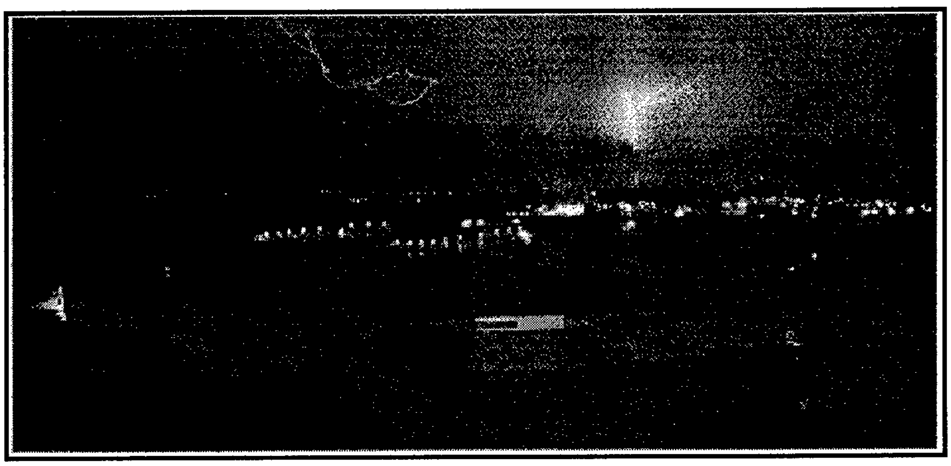
**Materials Analyses with Brilliant X-rays**

When completed in 1996, Argonne's Advanced Photon Source will generate the world's most brilliant synchrotron X-rays for materials research in a variety of fields. The CMT Division is part of a collaborative access team investigating possible synchrotron research activities suitable for the Advanced Photon Source. Team members include representatives from Amoco Corp., Notre Dame University, Northwestern University, Illinois Institute of Technology, and the University of Florida. A prominent goal is to develop capabilities to analyze environmentally relevant samples at a microscopic level never before possible.



*Advanced Photon Source under construction at Argonne. It will be the world's largest X-ray source. The Division plans to make extensive use of this facility in work on environmental and hazardous waste problems.*

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